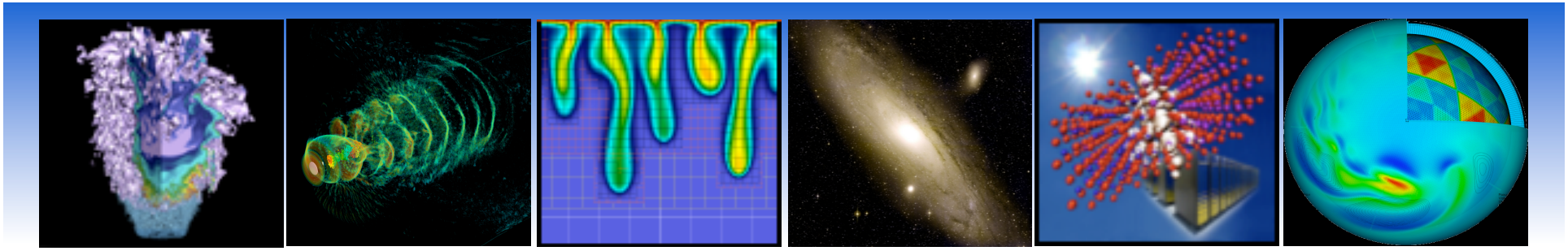

Building Transparent User Gateways at NERSC

Shreyas Cholia
NERSC/LBL

GlobusWorld, March 2nd 2010

Argonne National Laboratory

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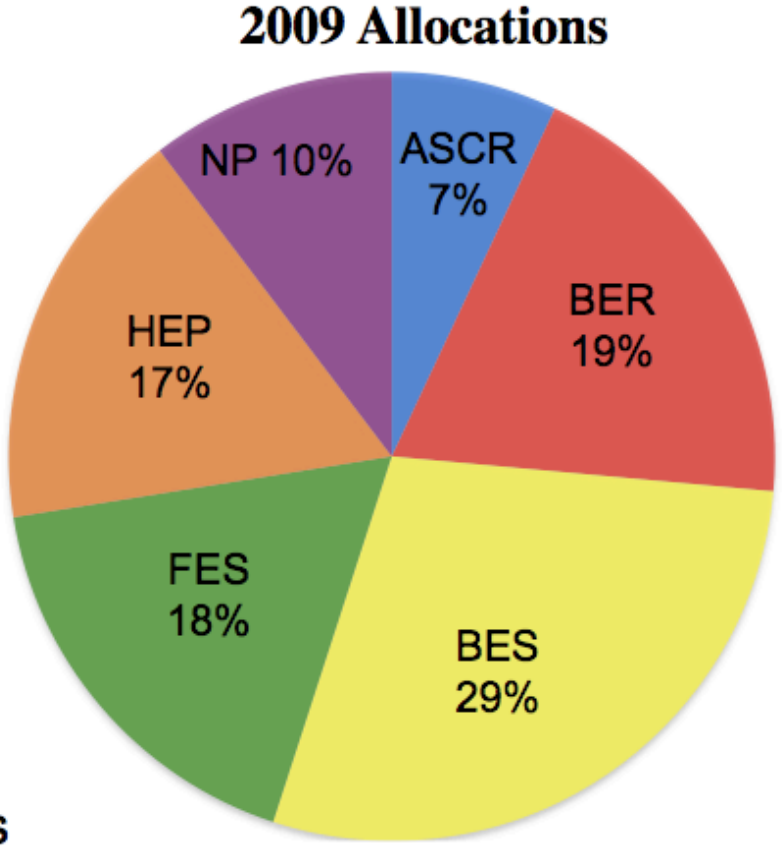
What is NERSC

- **National Energy Research Scientific Computing Center**
  - DOE Office of Science User Facility at Lawrence Berkeley National Laboratory
- **Mission:**
  - accelerate the pace of scientific discovery in the DOE Office of Science community by providing high-performance computing, information, data, and communications services.

NERSC is the Primary Computing Facility for the Office of Science

- NERSC serves a large population
  - Approximately 3000 users,
  - 400 projects, 500 code instances
- Focus on "unique" resources
  - –High end computing systems
  - –High end storage systems
    - File system and tape archive
  - –Interface to high speed networking
- Science-driven
  - –Science problems used in machine procurements and performance metrics
  - –Science services



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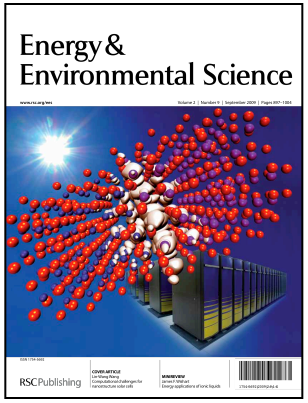
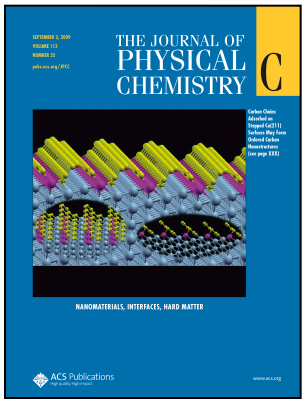
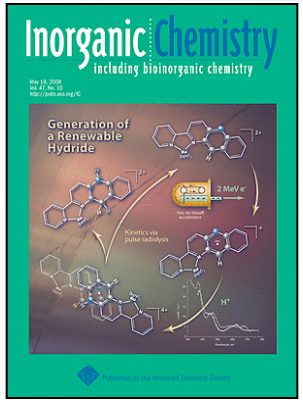
High quality science results from simulations of many different scales



64-6000 cores

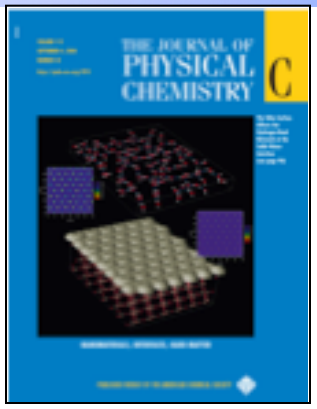


4-128 cores



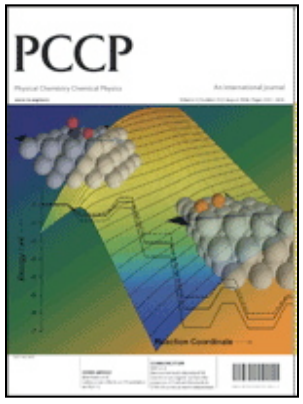
32 cores

1100-4600 cores

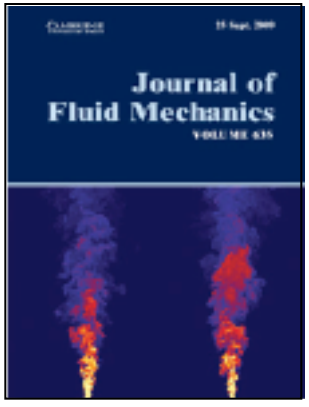


32-1024 cores

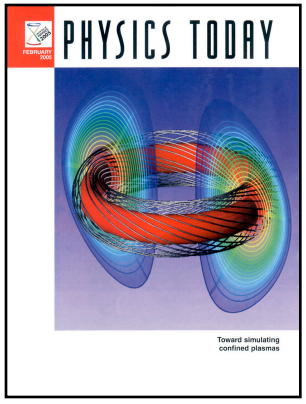
256 cores



32-256 cores



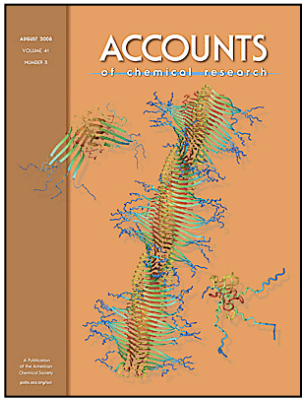
64-4096 cores



1000-4000 cores

80-260 cores

64-4700 cores



1100-4600 cores

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NERSC Cover Stories

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NERSC Systems

PDSF HEP Linux Cluster

Franklin Cray XT4

Hopper Cray XT5

DaVinci SGI Altix

Carver IBM IDataplex Cluster

Magellan IBM Idataplex Cloud

GPFS Global FS

HPSS Mass Storage

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Diversity of Users and Systems

- Users have differing application requirements
- Wide range of access patterns
- Multiple systems to meet different user needs

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Grid Usage

- **Open Science Grid has an allocation at NERSC – primarily for MPI users**
- **PDSF – STAR, ATLAS, ALICE, Planck using Grid tools to access system**
- **GridFTP – very popular for WAN data movement**
- **Grid certificate based workflow – very unpopular among wider user community ☹**
  - Managing certificates and dealing with existing CLI tools a huge deterrent for new users

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GSI is still Useful

- **As site admins and developers we see the value of the GSI infrastructure**
  - Provides a secure SSO to HPC resources
  - Common credential across multiple resources
  - Reduces password based access
  - Separates AuthN from AuthZ
  - Preserves user identity
- **How do we preserve these semantics without burdening the user?**

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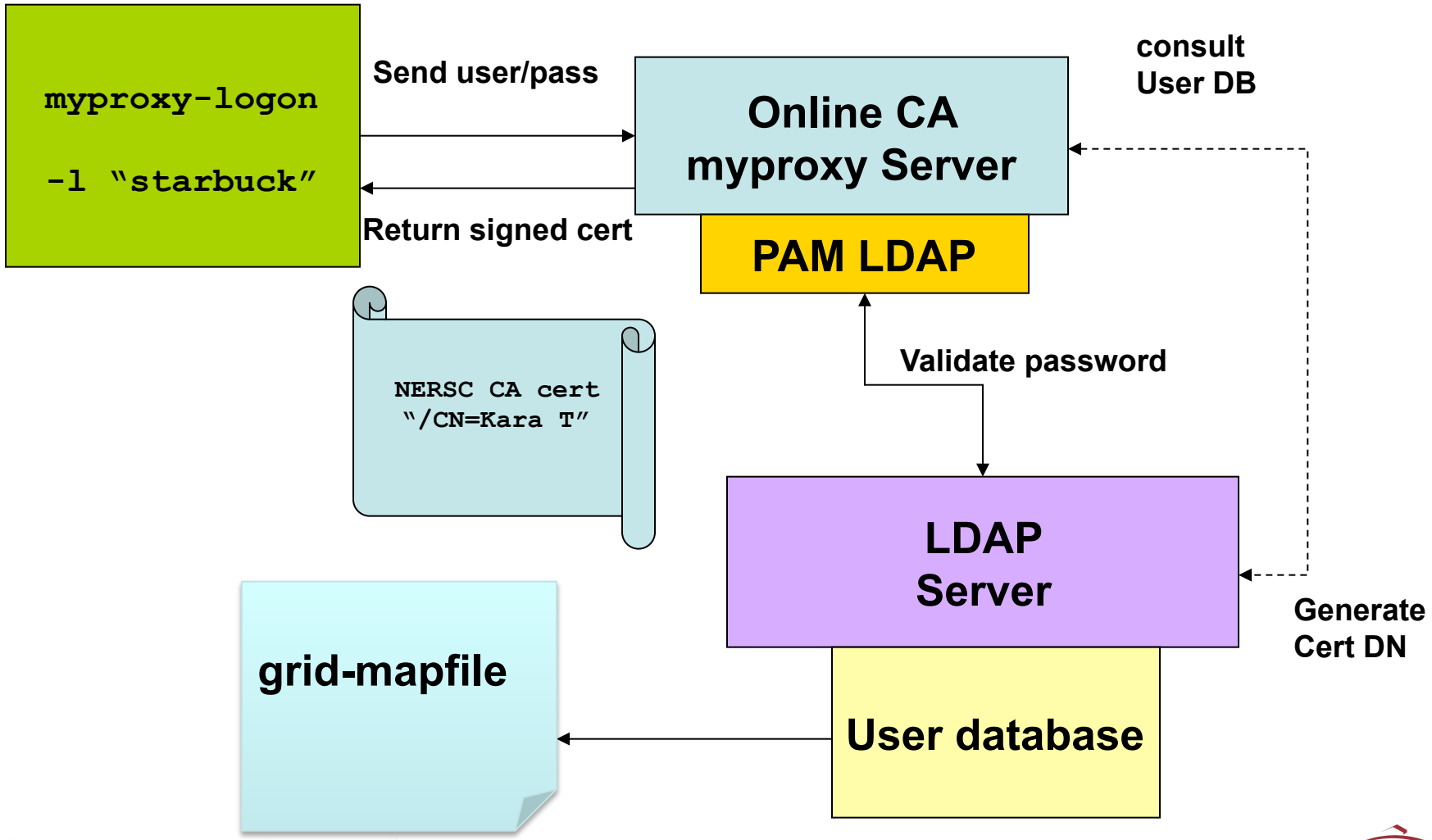
Step 1: Simplify Certificate Generation and Management

- **NERSC runs MyProxy in CA mode**
  - Single command to get a cert
  - Generates a brand new Short-lived cert based on username/password authentication
  - Backended to existing NERSC LDAP database
- **Generate persistent DNs AND populate grid-mapfiles on various systems using the same LDAP info**
  - Include example

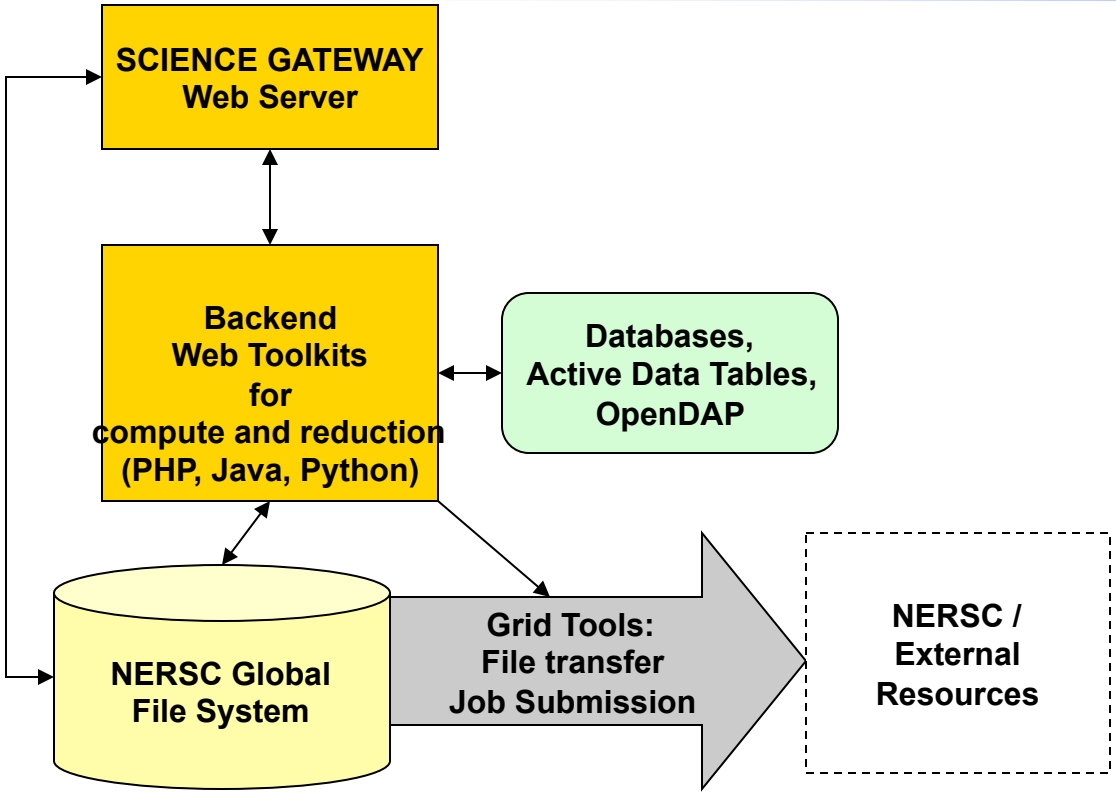
NERSC CA Service



Step 2: Hide Complexity through Web Gateways

- **Web access methods to NERSC resources**
- **Users very comfortable with web paradigm. Now expect it for usablity**
- **HPC should be as easy online-banking**
- **Custom gateways for individual science projects**
  - Users don't want to see generic options or tools not applicable to their science
  - Users don't want to deal with grid centric views
- **NERSC gateway services**
  - host the gateway
  - assist in building the webapp
  - provide building blocks to science groups for their own apps.

NERSC Science Gateways



Provide sophisticated building blocks for science on the web

- Direct access to massive data (NGF) through web-server
- Reduction and compute backend tools available (PHP, Python, Java)
- Databases, active tables, OpenDAP, File Browsing tools
- Grid tools for file transfer and job submission

Planck Gateway - Login

Computational Cosmology Center

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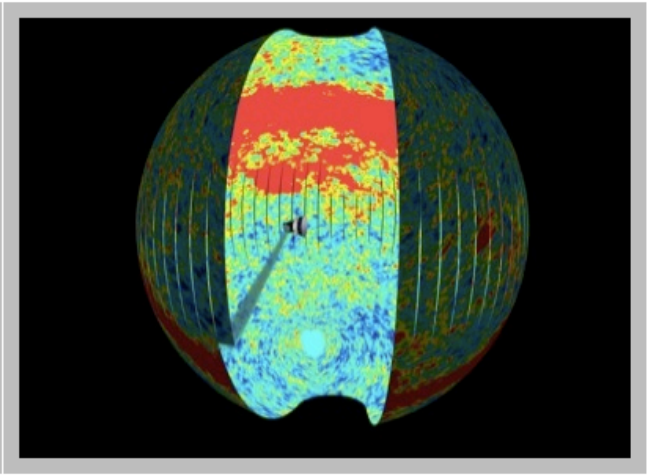

Username: shreyas

Password: ••••••••

Login

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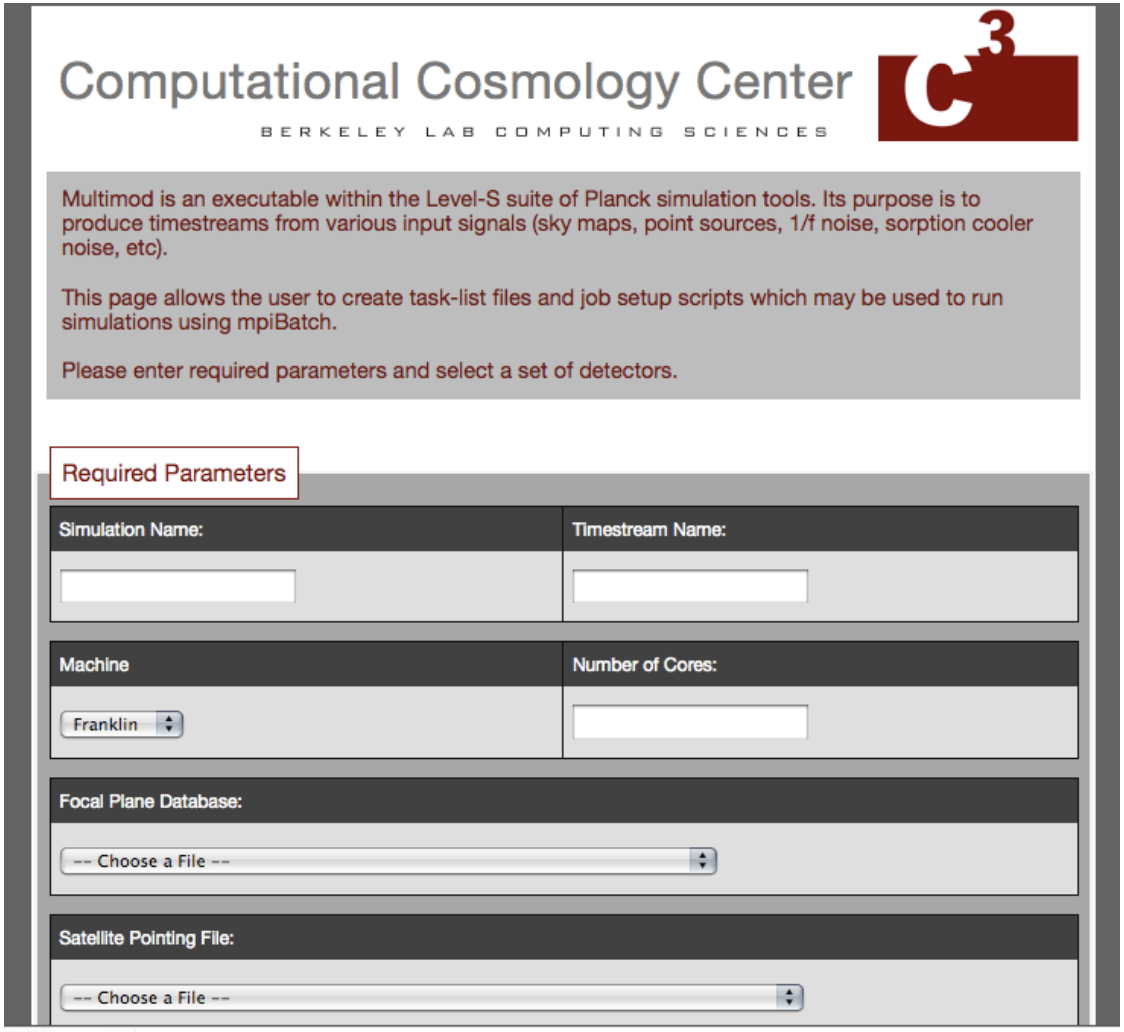
Planck Gateway – Web Application



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Benefits

- Perform actions on as the user on remote systems.
- User doesn't ever know about backend globus/GSI layer
- We preserve authorization at the infrastructure layer by using GSI certificates to access resources

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Currently

- **Set of ad-hoc portals**
  - DeepSky
  - Planck
  - GCRM (demo)
  - QCD
  - OpenDAP service for NETCDF data

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Step 3: Access Resources through Reusable Web API

- **Ad hoc approach has been productive but we see common patterns**
- **Encapsulate these patterns as building blocks for Science Gateways**
- **Building block API should be very easy to invoke eg. via a simple web page**
  - Every resource should be encapsulated as a URL with a simple set of associated actions

REST

- Representational State Transfer
- Every resource is represented by a unique http URL
- Actions are defined by standard HTTP methods: GET, POST, PUT, DELETE
- Think of it as an API that uses the language of HTTP
- NERSC Web Toolkit (NEWT) - RESTful service that provides access to NERSC resources
- NEWT combines NERSC database resources, Grid resources and other RESTful services under a single API

NEWT API examples

VERB	RESOURCE	DESCRIPTION
POST	/resource/job/	submit POST data to queue on R, return job id
GET	/resource/file/path/fname	get "fname" in "path" on R, copy it to apache server and download the file
GET	/user/username	get user account info

We are building this using the Django python framework. Authentication (MyProxy), File Transfer (GridFTP) and Job Management (GRAM) is completely transparent to the user and web application developer

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HPC as a Service

- Build web applications through REST API
- No need for science team to learn underlying framework
- GSI and globus calls essentially act at the backend protocol layer
- User interacts with a web application that exposes the necessary components of the underlying application

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In Development

- **Build reusable components and expose them through a REST API.**
- **Globus.org is very interesting this context**
  - Will provide us with a backend service layer to perform distributed computing tasks
  - Waiting for RESTful interface to service

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Thanks

Josh Boverhof

David Skinner

R.K. Owen

Contact: Shreyas Cholia

scholia@lbl.gov

Questions?

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